Amendments to the Claims

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims

1. (currently amended): A method for selecting at least one lead-candidate compound[[s]] capable of binding to a biopolymer, wherein the lead-candidate compound is a candidate for use as a physiologically active compound when the compound interacts specifically with the biopolymer, comprising:

obtaining ~~from~~ a compound database ~~containing three-dimensional structure~~ comprising information on atomic types and covalent bonds of compounds in the database,

selecting ~~of compounds by using a computer, wherein one or more~~ at least one query ~~compounds~~ molecule ~~which are assumed to be~~ capable of binding to ~~a receptor~~ the biopolymer, ~~or assumed to fit a virtual receptor model, or already known to be capable of binding to a receptor biopolymer are used as query molecules, structures of the compounds are modified to an extent that their binding to the biopolymer should not be retarded, and stability of complex structures of the biopolymer and the compounds is used as criteria for judgment~~

and selecting at least one trial compound by matching the at least one query molecule with trial compounds stored in the database based on information on atomic types and

covalent bonds of the at least one query molecule.

2. (currently amended): [[A]] The method of claim 1, further comprising modifying the structure of the at least one query molecule by an automatic structure construction method ~~for selecting lead-candidate compounds capable of binding to a biopolymer from a compound database containing three-dimensional structure information of compounds by using a computer, wherein one or more query compounds which are assumed to be capable of binding to a receptor biopolymer, or assumed to fit a virtual receptor model, or already known to be capable of binding to a receptor biopolymer are used as query molecules, structures of the compounds are modified to an extent that their binding to the biopolymer should not be retarded, stability of complex structures of the biopolymer and the compounds is used as criteria for judgment, and characterized by a first screening based on quantitative information including number of atoms and the like, a second screening based on information about atomic types and mode of covalent bonds, and a third screening based on structures of complexes formed with the biopolymer based on correspondence of atoms with those of the query molecules~~.

3. (currently amended): [[A]] The method of claim 1, wherein the matching of the at least one query molecule is performed by judging similarity of partial structures based on two-dimensional graphs where each atom is represented as a node and each covalent bond is represented as an arc ~~for selecting lead-candidate compounds~~

~~capable of binding to a receptor biopolymer from a database containing, at least, information about atomic types and mode of covalent bonds of compounds by using a computer, which comprises the following step:~~

~~(a) a step of selecting lead-candidate compounds by matching one or more query molecules capable of binding to a biopolymer with compounds stored in a database based on information about atomic types and mode of covalent bonds of the query molecules~~.

4. (currently amended): The method of claim 3 wherein the ~~database contains information about three-dimensional structure of the compounds~~ matching of the at least one query molecule is performed by the algorithm of Ullman.

5. (currently amended): The method of claim 3 ~~which comprises~~ further comprising ~~a step (b) of~~ screening the trial compounds based on information on marker sites in the ~~constructing structures of the~~ query ~~compounds by an automatic structure construction method~~ molecules.

6. (currently amended): The method of claim [[3]] 1, further comprising ~~wherein the step (a) comprises either or both of the following two steps~~:

~~(c) a step of first screening by selection of trial compounds based on one or more parameters selected from a group of parameters consisting at least of number of atoms, number of bonds, number of ring structures, number of atoms for each atomic~~

~~type and molecular weight~~

estimating binding schemes of the trial compounds to the biopolymer based on the binding schemes of at least one query molecule to the biopolymer; ~~and/or~~

calculating at least one parameter relating to interaction between the trial compounds and the biopolymer; and

~~(d) a step of second~~

screening the trial ~~by matching of candidate~~ compounds ~~selected in the first screening step for mode of covalent bonds~~ based on the parameters.

7. (currently amended): The method of claim ~~6~~ 1, further comprising ~~wherein the step (d) comprises the following step~~:

~~(e) a step of second screening based on information about marker sites in the query molecules~~

estimating a virtual receptor model which represents physicochemical environment of the ligand binding site of the biopolymer based on information of three-dimensional structures of one or more known ligands capable of binding to the biopolymer;

judging goodness of fit of the trial compounds to the virtual receptor model; and

screening the trial compounds based on the goodness of fit.

8. (currently amended): The method of claim [[3]] 1, further comprising ~~wherein, after the step(a), a third~~ screening ~~is performed by the following step (f):~~

~~(f) a step of selecting one or more preferred lead-candidate~~ trial compounds ~~by estimating binding schemes to the biopolymer for the lead-candidate compounds selected in the step (a)~~ based on ~~three-dimensional information and binding schemes of the query molecules to the biopolymer, and calculating~~ at least one ~~or more parameters~~ parameter selected from number of atoms, number of bonds, number of ring structures, number of atoms for each atomic type, and molecular weight ~~relating to interaction between the lead-candidate compounds and the biopolymer;~~

~~and/or the following step (g):~~

~~(g) a step of selecting one or more preferred lead-candidate compounds by supposing a virtual receptor model which represents physicochemical environment of the ligand binding site of the biopolymer based on information of three-dimensional structures of one or more known ligands capable of binding to the biopolymer, and then judging goodness of fit to the virtual receptor model for the lead-candidate compounds selected in the step (a)~~.

9. (new) The method of claim 1, further comprising calculating the interaction energy between the at least one trial compound and the biopolymer.

10. (new) A method for selecting at least one lead-candidate compound capable of binding to a biopolymer from a compound database comprising information on atomic types and covalent bonds of compounds in the database, comprising selecting at least one trial compound by matching at least one query molecule capable

of binding to the biopolymer with trial compounds stored in the database based on information on atomic types and covalent bonds of the at least one query molecule.